Direct Simulation of Hydrodynamically Unstable Premixed Flames

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11th International Workshop on Premixed Turbulent Flames
McGill University

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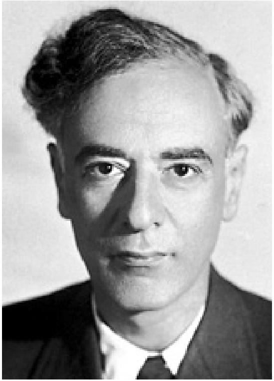
[1] Thanks to M. Matalon for helpful discussions.

Outline

Hydrodynamic[2] Instability

Lev Landau



1908 – 1968

Georges Darrieus

1888 – 1979

[2] Also Landau-Darrieus, Darrieus-Landau, and Thermo-Expansive

Hydrodynamic[2] Instability

Lev Landau

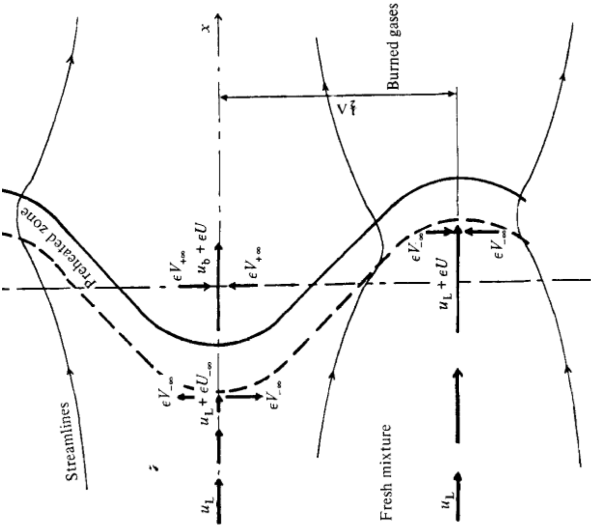
Physics, 1962

Georges Darrieus

1888 – 1979

[2] Also Landau-Darrieus, Darrieus-Landau, and Thermo-Expansive

Non-Mathematical Explanation



“quasi-incompressible fluid + reaction front ⇒ instability”

Darrieus' and Landau's Analysis (1930's and 40's)

Imagine a flame in the x-y plane. Assuming

- The flame is infinitely thin
- Fluid satisfies Euler equations on either side of the flame
- Flame expands the volume by the factor $\mathcal{R}$
- Local flame speed is s_0
- Flame location is $y = c\exp(\omega t)\cos(kx)$

then

$$\omega_{\mathrm{LD}} = \frac{\sqrt{\mathcal{R}^3 + \mathcal{R}^2 - \mathcal{R}} - \mathcal{R}}{\mathcal{R} + 1}\, s_0\, k$$

Since $\omega_{\mathrm{LD}} > 0$ whenever $\mathcal{R} > 1$, the instability is *unconditional*.

Markstein's Analysis (1951)

Assuming as before, except

- Local flame speed is $s = s_0(1 - \mathcal{L}\kappa)$

then

$$\omega_{\mathrm{Ma}} = \frac{\sqrt{\mathcal{R}^3(1-2\mathcal{L}k) + \mathcal{R}^2(1+\mathcal{L}^2k^2) - \mathcal{R}} - \mathcal{R}(1+\mathcal{L}k)}{\mathcal{R}+1}\, s_0\, k\,.$$

In this case $\omega_{\mathrm{Ma}} > 0$ only when

$$\mathcal{R} > 1 \quad \text{and} \quad \mathcal{L} < 0 \quad \text{and} \quad k < k_c\,, \quad \text{where} \quad k_c = \frac{\mathcal{R}-1}{2\mathcal{L}\mathcal{R}}\,.$$

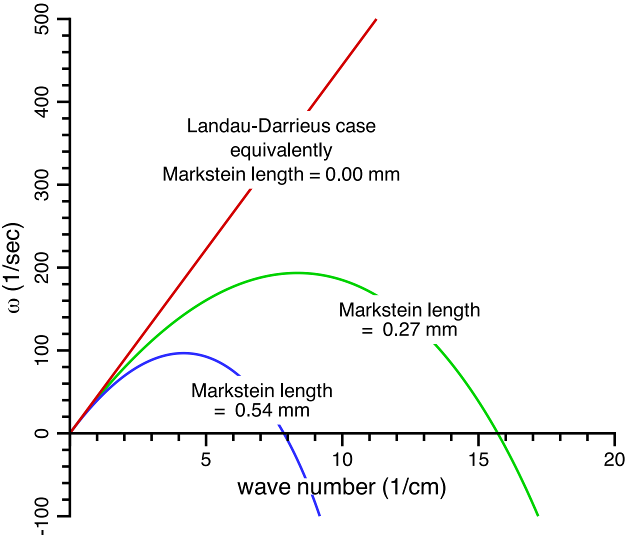
Corresponding to the critical wavenumber k_c is the critical wavelength $\lambda_c = 2\pi/k_c$ above which amplification occurs.

So, more realistically, only perturbations with sufficiently long wavelengths are predicted to be unstable.

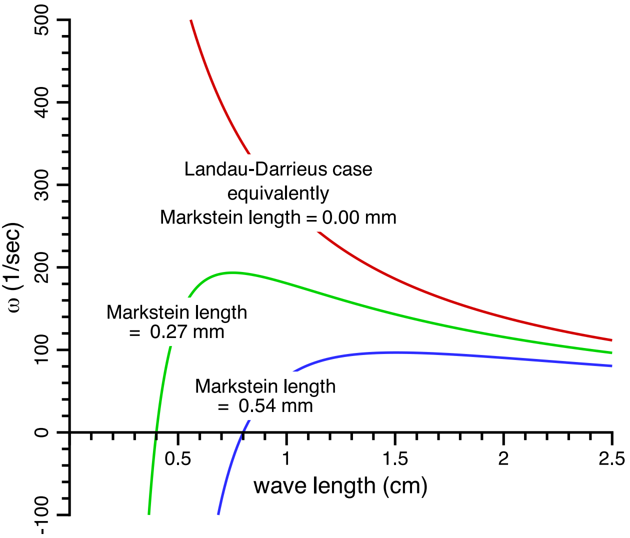
Specific Methane-Air Flame

mechanism	DRM19
ϕ	0.8
α_0	2.24 cm^2/s
$\mathcal{L}$	
Le	0.96
Pr	0.72
$\mathcal{R}$	6.68
s_0	29.27 cm/s
T_0	300 K
T_a	17207 K

Dispersion Relation



Dispersion Relation with Respect to Wavelength



Kuramoto-Mickelson-Sivashinsky Equation (1977)

Thermo-diffusive instability discovered by Zeldovich (1944):

- Analyzed by Zeldovich, Barenblatt, and Sivashinsky
- Assuming $\mathcal{R} = 1$ (“constant density approximation”)
- Instability requires $\mathrm{Le} < \mathrm{Le}_c < 1$

Sivashinsky (1977) combined -diffusive and -expansive effects:

- Assuming $\mathcal{R} \approx 1$ (“weak thermal limit”)
- Assuming $\mathrm{Le} \approx \mathrm{Le}_c$
- For $\mathcal{R} = 1$ there is a nonparametric evolution equation, the K-M-S equation, with dozens of physical applications
- For $\mathcal{R} \neq 1$ and $\mathrm{Le} = 1$ *another* nonparametric equation describes the purely hydrodynamic instability

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial \xi^2} - \frac{1}{2}\left(\frac{\partial u}{\partial \xi}\right)^2 + \frac{1}{2\pi}\int_0^\infty \int_{-\infty}^\infty k\, u(x,\tau) \cos k(\xi - x)\, dx\, dk$$

More Realistic Assumptions (1982)

Three papers

1. Pelce and Clavin
2. Matalon and Matkowsky
3. Frankel and Sivashinsky

- Assuming one irreversible reaction
- Assuming no restrictions on Le and $\mathcal{R}$
- All found viscosity has no effect
- All have different notation and nondimensionalizations

$$\omega_{FS} = \frac{\sqrt{\mathcal{R}^3+\mathcal{R}^2-\mathcal{R}}-\mathcal{R}}{\mathcal{R}+1} s_0\, k + \left[\frac{\mathcal{R}^2 \log\left(\frac{\mathcal{R}^2+2\sqrt{\mathcal{R}^3+\mathcal{R}^2-\mathcal{R}}+1}{\mathcal{R}^2(\mathcal{R}+1)}\right) - (\mathcal{R}-1)^2}{2(\mathcal{R}-1)\sqrt{\mathcal{R}+1-\mathcal{R}^{-1}}} \right.$$

$$\left. + \frac{\mathcal{R}\left(\sqrt{\mathcal{R}^3+\mathcal{R}^2-\mathcal{R}}+\mathcal{R}+2\right)+\sqrt{\mathcal{R}+1-\mathcal{R}^{-1}}-1}{2(\mathcal{R}+1)^2\sqrt{\mathcal{R}^3+\mathcal{R}^2-\mathcal{R}}} \mathrm{Li}_2(1-\mathcal{R}) \frac{T_a}{T_0}(\mathrm{Le}-1) \right] \alpha_0\, k^2$$

F & S predict unrealistically small $\lambda_c = 0.079$ cm

Matalon, Cui, and Bechtold (2003)

New analysis

- Assuming properties vary through the flame zone
- Viscous terms do not drop out

$$
\begin{aligned}
\omega_{\mathrm{MCB}} \quad = \quad & \frac{\sqrt{\mathcal{R}^3+\mathcal{R}^2-\mathcal{R}}-\mathcal{R}}{\mathcal{R}+1}\, s_0\, k \\
& - \left[\frac{\mathcal{R}\left(3\mathcal{R}^3+\mathcal{R}^2+4\sqrt{\mathcal{R}^3+\mathcal{R}^2-\mathcal{R}}\mathcal{R}+\mathcal{R}-1\right)}{4(\mathcal{R}+1)\sqrt{\mathcal{R}^3+\mathcal{R}^2-\mathcal{R}}} \right. \\
& + \frac{T_a}{T_0}(\mathrm{Le}_{eff}-1)\frac{(\mathcal{R}-1)^2\left(\sqrt{\mathcal{R}^3+\mathcal{R}^2-\mathcal{R}}+1\right)\left(\mathcal{R}^2+\sqrt{\mathcal{R}^3+\mathcal{R}^2-\mathcal{R}}\right)}{2\mathcal{R}(\mathcal{R}+1)^2\sqrt{\mathcal{R}^3+\mathcal{R}^2-\mathcal{R}}} \\
& \left. + \Pr \frac{(\mathcal{R}-1)^2\mathcal{R}}{2\sqrt{\mathcal{R}^3+\mathcal{R}^2-\mathcal{R}}} \right] \alpha_0\, s_0\, k^2
\end{aligned}
$$

M C & B predict realistic $\lambda_c = 0.48$ cm

Outline

DNS Requirements to Study Natural Flames

1. **Spatial resolution** requirement:

   13 points through the flame zone.

   flame zone thickness 0.2 mm $\Rightarrow$ spatial resolution $\Delta x \approx 15\mu$

2. **Temporal duration** requirement:

   The flame must traverse, chemically, a significant distance to reveal its natural behavior.

   $$\text{total time} = \frac{60 \times \text{thermal thickness 0.5 mm}}{\text{flame speed 29 cm/s}} = 0.1 \text{ sec}$$

3. **Temporal resolution** requirement (CFL stability condition):

   $$\Delta t < 0.5 \times \frac{\Delta x}{\text{fastest speed in simulation}}$$

4. **Number of time steps** required

   $$N = \frac{\text{total time}}{\Delta t} > \frac{0.2 \text{ fastest speed}}{\Delta x} = 13,500 \times \begin{array}{c}\text{fastest}\\ \text{speed (m/s)}\end{array}$$

Traditional DNS versus low Mach number DNS

$$\begin{aligned} \text{time steps } N &= 13{,}500 \times \text{fastest speed in simulation(m/s)} \\ \text{traditional DNS} &= \ldots \times \text{sound speed at 2000 K} = 10{,}400{,}000 \\ \text{low Mach-number} &= \ldots \times \text{hot gas velocity} \qquad = 27{,}500 \end{aligned}$$

A flame must traverse a significant distance, as a result of chemical reactions, to reveal its natural behavior.

This work uses the low Mach-number combustion software developed at Lawrence Berkeley National Laboratory (LBNL).

- low Mach-number formulation
- adaptive mesh refinement (AMR)
- mixture-averaged transport without cross-diffusion implemented by Day and Bell (2000)

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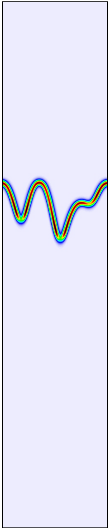
Computational Setup



initial fuel mass consumption

Freely propagating 2D flame

- CH_4-Air with $\phi = 0.8$
- No gravity
- No radiation losses
- Widths 0.4, 0.8, and 1.2 cm
- $0.1+$ seconds duration

- Initially randomly wrinkled flame
- Bottom inflow controlled to hold flame steady
- Side boundaries periodic
- Aspect ratio height:width $= 5 : 1$
- Controlled inflow

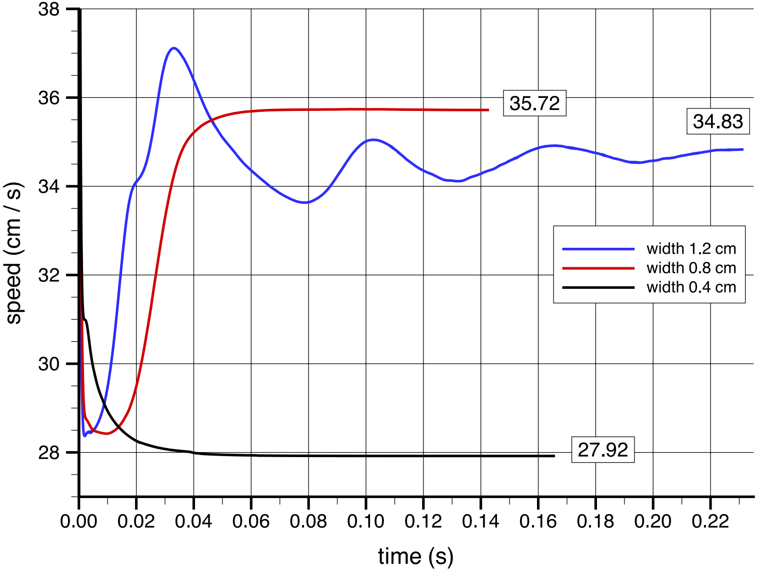
Movies

0.4 cm

0.8 cm

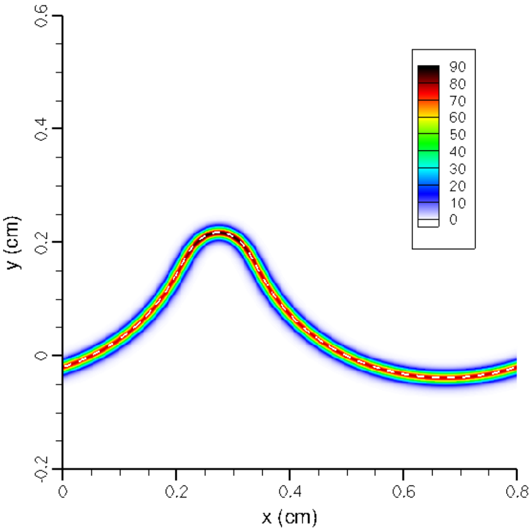
1.2 cm

Flame Speed

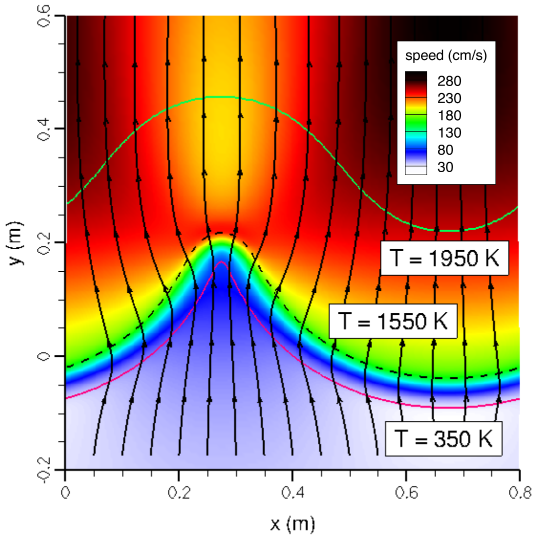


38
36
34
32
30
28
speed (cm / s)
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
0.18
0.20
0.22
time (s)
35.72
34.83
27.92
width 1.2 cm
width 0.8 cm
width 0.4 cm

Fuel Consumption Isotherm

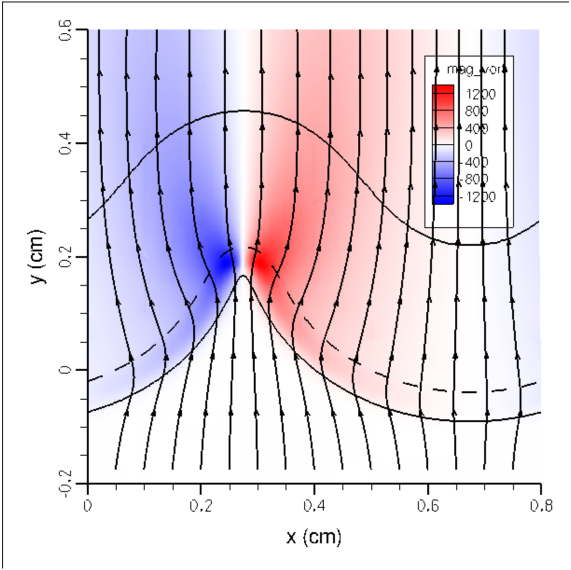


Velocity



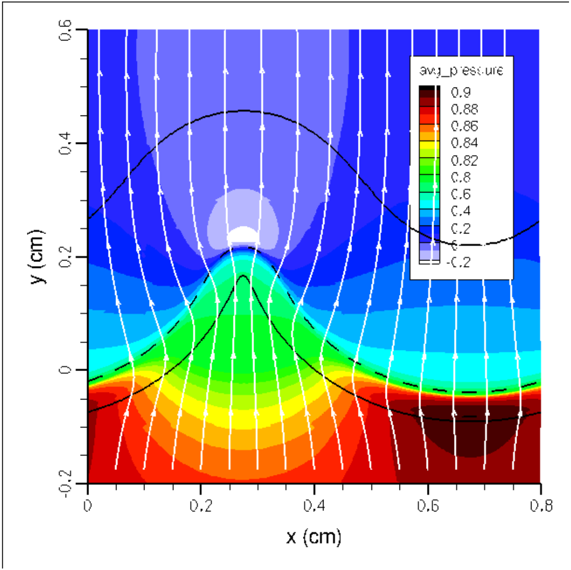
speed (cm/s)
280
230
180
130
80
30
T = 1950 K
T = 1550 K
T = 350 K
y (m)
x (m)
0.6
0.4
0.2
0
-0.2
0
0.2
0.4
0.6
0.8

Vorticity



mag_vort
1200
800
400
0
-400
-800
-1200
y (cm)
0.6
0.4
0.2
0
-0.2
x (cm)
0
0.2
0.4
0.6
0.8

Pressure



avg_pressure
0.9
0.88
0.86
0.84
0.82
0.8
0.6
0.4
0.2
-0.2
y (cm)
0.6
0.4
0.2
0
-0.2
0
0.2
0.4
0.6
0.8
x (cm)

Outline

Summary

- Theory has evolved to the point that Matalon et al (2003) appear to give quantitatively correct predictions
- The non-mathematical explanation of Landau appears to most accurately describe the instability
- Contrary to previous simulations, the flame appears *not* susceptible to “jitters” once it assumes the canonical shape.
- As the simplest nontrivial flame, it may be used to test many theorized relationships. Suggestions welcome.

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